Negative superdiffusion due to the inhomogeneous convection

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Fractional transport of particles on a comb structure in the presence of an inhomogeneous convection flow is studied. The large scale asymptotics is considered. It is shown that a contaminant spreads superdiffusively in the direction opposite to the convection flow. Conditions for the realization of this new effect is discussed in detail.

A realization of superdiffusion on a subdiffusive media, *e.g.* on a comb structure [1], is an example of the fractional transport due to the inhomogeneous convection. These studies of the space–time evolution of an initial profile of particles in a specific media due to the inhomogeneous convection flow are arisen in a variety of applications such as transport of external species (pollution) in water flows through porous geological formations [2, 3], problems of diffusion and reactions in porous catalysts [4] and fractal physiology [5]. The conditions for the inhomogeneous convection which is responsible for the superdiffusive spreading of an initial packet of particles have been found in [1]. A classification of possible scenarios of the space–time evolution of a contaminant in the presence of the inhomogeneous convection on the comb structure is presented there. The external forcing has been taken in the power–law form for the convection current $j_x(t,x,y) = vx^s\delta(y)G(t,x,y)$, where a distribution $G(t,x,y)$ describes the evolution of the initial profile, while $vx^s\delta(y)$ is the inhomogeneous convection velocity. When $s < 0$ subdiffusion is observed [6, 7]. When $s > 0$ it is superdiffusion. The homogeneous convection with $s = 0$ corresponds formally to the normal diffusion, but the effective diffusion coefficient is determined by the external forcing v [1]. The frontier case with $s = 1$ corresponds to the log–normal distribution of transport particles, where one deals with not a sum of independent random variables but with their multiplication [8]. When $s > 1$ the fractional transport corresponding to superdiffusion possesses specific features. This case is the main subjective for the investigation in the present Letter. We consider both the fractional transport on the comb structure, where the number of transporting particles is not conserved, and the continuous time random walk (CTRW) with conservation of the total number of particles (transporting or not). This case of $s > 1$ differs essentially from those with $s \leq 1$ where the transporting particle move in the direction of the convection current j_x [1]. Unlike our previous consideration [1] in the present study we observed analytically that an asymptotic solution for the transporting particles corresponds to superdiffusion in the direction opposite to the convection flow current $-j_x$. This is a result of an irreversible relaxation process [9] which is "inevitable" process in the diffusion transport phenomena.

First, we will describe the superdiffusion on the comb structure due to the inhomogeneous convection described by the $2D$ distribution function $G = G(t,x,y)$ and the current

$$\mathbf{j} = \left(v(x,y)G - \tilde{D}\delta(y)\frac{\partial G}{\partial x}, -D\frac{\partial G}{\partial y} \right), \qquad (1)$$

where $\tilde{D}\delta(y)$ and D are the diffusion coefficients for the x and y directions correspondingly, while the inhomogeneous convection velocity is $v(x,y) = v|x|^s\delta(y)$.

The comb model is known as a toy model for porous media used for the exploration of low dimensional percolation clusters [10] and an electrophoresis process [11]. For $v = 0$ subdiffusion have been observed [12]. A special transport behavior on the comb structure is that the displacement in the x–direction is possible only along the structure x-axis, say at $y = 0$, according to Eq. (1). Both the diffusion coefficient and the convection flow are highly inhomogeneous in the y-direction. There is also diffusion in the y–direction with a constant diffusion coefficient D. Therefore the Liouville equation

$$\frac{\partial G}{\partial t} + \mathrm{div}\,\mathbf{j} = 0$$

corresponds to the following Fokker–Planck equation

$$\frac{\partial G}{\partial t} + \hat{L}_{FP}(x)G\delta(y) - D\frac{\partial^2 G}{\partial y^2} = 0 \qquad (2)$$

with the Fokker–Planck operator of the form

$$\hat{L}_{FP}(x)G = -\tilde{D}\frac{\partial^2 G}{\partial x^2} + v|x|^s\frac{\partial G}{\partial x} + sv|x|^{s-1}\mathrm{sgn}\,(x)G.$$

The initial condition is $G(0,x,y) = \delta(x)\delta(y)$, and the boundary conditions on the infinities have the form $G(t,\pm\infty,\pm\infty) = 0$ and the same for the first derivatives with respect to x and y $G'_x(t,\pm\infty,\pm\infty) = G'_y(t,\pm\infty,\pm\infty) = 0$. The function $\mathrm{sgn}\,(x)$ equals to 1 for $x > 0$ and -1 for the opposite case. The transport of particles along the structure x-axis is described by the function $G(t,x,y = 0) = g(x,t)$. It should be underlined that the tails of the distributions are the most interesting for applications. Therefore, we are studying here the large scale asymptotics when $|x| \gg 1$. In

the Laplace–Fourier ($\mathcal{LF}$) space (p, k) Eq. (2) is transformed to the following fractional equation for the function $\tilde{g} = \tilde{g}(p, k) = \mathcal{LF}[g(t, x)]$

$$\tilde{D}k^2\tilde{g}(p, k) + ik\frac{\partial^s\tilde{g}(p, -k)}{\partial|k|^s} + 2\sqrt{D}p\tilde{g}(p, k) = 1 . \quad (3)$$

Here the fractional Reisz derivative is the result of the Fourier transform [9, 13]

$$-\frac{\partial^s\tilde{g}(\ldots, -k)}{\partial|k|^s} = \mathcal{F}[|x|^s g(\ldots, x)] .$$

The large scale asymptotics $|x| \gg 1$ corresponds to $|k| \ll 1$ in the Fourier space. Therefore, the first term in (3) can be omitted at the condition

$$\lim_{\substack{k \to 0 \\ p \to 0}} \frac{k^2}{p^{1/2}} = 0 . \quad (4)$$

This approximation depends on the form of singularity of the the convection velocity in the limit $x \to \infty$. It means that the asymptotic solutions of the homogeneous part of Eq (3) for $|x| \gg 1$ depends on the exponent s in the power law $|x|^s$ [14, 15]. After performing the inverse Fourier transform, one obtains the asymptotic of $x \gg 1$ solution that corresponds to the homogeneous part of Eq. (3). It reads

$$\tilde{g}(p, x) = \frac{1}{|x|^s}\exp\left[\frac{2\sqrt{Dp}|x|^{1-s}\text{sgn}(x)}{(s-1)v}\right] . \quad (5)$$

This solution describes asymptotic transport of any initial profile. To obtain the time–dependent solution one carries out the inverse Laplace transform $g(t, x) = \mathcal{L}^{-1}[\tilde{g}(p, x)]$. The necessary condition theorem needs the negative sign of the function in the exponential in Eq. (5). It depends only on s and the sign of v. When $s < 1$, the initial profile of particles moves in the directions of the convection flow, namely, in the direction of $v = |v|$ for $x > 0$, and $v = -|v|$ for $x < 0$. It is usual superdiffusive acceleration of diffusion due to the inhomogeneous convection. This case together with $s = 1$ was considered in detail in [1].

When $s > 1$ the situation is much interesting and leads to the absolutely new effect. Indeed, for $s > 1$, the necessary condition to perform the inverse Laplace transform is $v = -|v|$, when $x > 0$ and $v = |v|$, when $x < 0$. Hence, the inverse Laplace transform gives

$$g(t, x) = \frac{-\text{sgn}(x)D^{1/2}|x|^{1-2s}}{v(s-1)\sqrt{\pi t^3}}\exp\left[-\frac{Dx^{2-2s}}{v^2(s-1)^2 t}\right] . \quad (6)$$

When $|x| \gg 1$ and t is large enough to put the exponential to the unite, one obtains the distribution for superdiffusion of particles

$$g(t, x) \propto \frac{1}{|x|^{2s-1}\sqrt{\pi t^3}} . \quad (7)$$

All moments of x higher than $2s - 2$ are equal to the infinity. It also should be underlined that the flux on the infinities is vanishing. The important feature of this superdiffusion is that it occurs in the direction opposite to the inhomogeneous convection current. This new phenomenon is related to the relaxation process or it is due to diffusion, where the Kolmogorov conditions (see [9]) are necessary for the inferring of the Fokker–Plank equation (FPE). In the absence of the convection the solution of the FPE gives that at any moment $t > 0$ the particles are spread over the all x–axis from the minus infinity to the plus infinity with the exponentially small tails. It is correct not only for the normal diffusion but for the subdiffusive relaxation on the comb structure, as well [12]

$$g(t, x) = \frac{\tilde{D}}{2\pi\sqrt{Dt^3}}\int_0^\infty \exp\left[-\frac{x^2}{4\tilde{D}u} - \frac{Du^2}{t}\right]u^{1/2}du .$$

This behavior is dominate for small x even in the presence of the inhomogeneous convection. But for the asymptotically large x the inhomogeneous convection in the direction opposite to the spreading of particles changes the shape of the tail of the packet from the exponential to the power law in according with Eq. (7). We call this solution the negative superdiffusion solution or the negative superdiffusion approximation (NSA).

The total number of transporting particles on the structure axis decreases with time

$$\langle G \rangle = \int_{-\infty}^\infty g(t, x)dx = (4s - 3)/\sqrt{\pi Dt} . \quad (8)$$

Therefore, the distribution function (6) describes the NSA when the number of particles $\langle G \rangle$ is not conserved. The formulation of the NSA problem with conservation of the total number of particles is equivalent to the case with a continuous distribution of the delay times [8], where the total number of particles is described by the function $G_1(t, x) = \int_{-\infty}^\infty G(t, x, y)dy$. It is simply to show from Eq. (2) that

$$G(t, x, y) = \mathcal{L}^{-1}\left[\tilde{g}(p, x)e^{-\sqrt{p/D}|y|}\right] . \quad (9)$$

Taking this into account, one obtains the equation for G_1 by integrating Eq. (2) with respect to the y variable. It reads in the Laplace space for $\tilde{G}_1(p, x) = \mathcal{L}[G_1(t, x)]$:

$$p\tilde{G}_1(p, x) + \hat{L}_{FP}(x)\tilde{g}(p, x) = \delta(x) \quad (10)$$

It is simply to see from Eq. (2) or Eq. (3) that

$$\hat{L}_{FP}\tilde{g}(p, x) = \delta(x) - 2\sqrt{pD}\tilde{g}(p, x) .$$

Substituting this in Eq. (10), one obtains that

$$\tilde{g}(p, x) = \frac{1}{2}\sqrt{p}D\tilde{G}_1(p, x) .$$

After substitution of this relation in Eq. (10), the CTRW equation in the Laplace space is

$$p^{1/2}\tilde{G}_1 + \frac{1}{2D}\hat{L}_{FP}(x)\tilde{G}_1 = p^{-1/2}\delta(x) . \quad (11)$$

We introduce the Riemann–Liouville fractional derivatives (see, for example, [7, 16]) $\frac{\partial^\alpha}{\partial t^\alpha} f(t)$ by means of the Laplace transform $(0 < \alpha < 1)$:

$$\mathcal{L}[\frac{\partial^\alpha}{\partial t^\alpha} f(t)] = p^\alpha \tilde{f}(p) - p^{1-\alpha} f(O^+) \qquad (12)$$

that also implies $\partial^\alpha[1]/\partial t^\alpha = 0$ [16]. Using this definition, we write down the CTRW equation which corresponds to the comb model desribed by Eq. (2)

$$\frac{\partial^{1/2} G_1}{\partial t^{1/2}} + \frac{1}{2D} \hat{L}_{FP}(x) G_1 = 0. \qquad (13)$$

Here the initial condition is $G_1(0, x) = \delta(x)$. For the asymptotically large scale $x \gg 1$ (or $x \ll -1$), we neglect the inhomogeneous term together with the second derivatives with respect to x in Eq. (11) to obtain the following equation

$$v(d|x|^s \tilde{G}_1/dx) + 2Dp^{1/2}\tilde{G}_1 = 0$$

with the NSA related to the CTRW by

$$\frac{1}{x^s} \exp\left[\frac{2Dp^{1/2} x^{1-s} \operatorname{sgn}(x)}{v(s-1)}\right]. \qquad (14)$$

In the rest of the Letter we infer the NSA in the framework of the Liouville–Green asymptotic solution for linear differential equations [15]. We show that the performed approximation due to the condition (4) is satisfactory good and corresponds to the Liouville–Green (LG) approximation also called the WKB approximation [17]. The CTRW equation (13) in the generalized form reads

$$\frac{\partial^\alpha G_1}{\partial t^\alpha} + \frac{1}{2D} \hat{L}_{FP}(x) G_1 = 0, \qquad (15)$$

where $0 < \alpha < 1$. Hence, for $x \gg 1$, we obtain the homogeneous part (lhs) of Eq. (11), where the item $p^{1/2}$ is substituted by p^α. It reads

$$-\tilde{G}_1'' + \frac{v}{\tilde{D}} x^s \tilde{G}_1' + \frac{vs}{\tilde{D}} x^{s-1} \tilde{G}_1 + p^\alpha \tilde{G}_1 = 0. \qquad (16)$$

The term in the first derivative is removed from the equation by the substitution

$$\tilde{G}_1 = \exp[vx^{s+1}/2\tilde{D}(s+1)]w. \qquad (17)$$

Thus $w'' = R(x)w$, where

$$R(x) = \frac{v^2 x^{2s}}{4\tilde{D}^2}[1 + \frac{2s\tilde{D}}{v} x^{-s-1} + \frac{8D\tilde{D}}{v^2} p^{1/2} x^{-2s}].$$

The LG approximation for w, that satisfies to the accepted boundary conditions (see Eq. (2)), is

$$w = BR^{-1/4} \exp\left[-\int R^{1/2} dx\right]$$

$$= B\sqrt{\frac{|v|}{2\tilde{D}}} \frac{1}{x^s} \exp\left[-\frac{vx^{s+1}}{2\tilde{D}(s+1)} - \frac{2Dp^\alpha x^{1-s}}{v(s-1)}\right], \qquad (18)$$

where B is a constant. Analogously, we obtain the LG solution for the negative $x \ll -1$. Therefore, taking $B = \sqrt{\frac{2\tilde{D}}{|v|}}$ and $\alpha = 1/2$, we obtain that Eq. (18) coincides exactly with the solution (14). It means that removing the second derivatives from $\hat{L}_{FP}$ or, the same, the term k^2 in the Fourier space in the limit $k \to 0$ corresponds to the Liouville–Green approximation for the Fokker–Planck equation with inhomogeneous (superdiffusive) convection. This asymptotic solution is superdiffusive transport of particles in the direction opposite to the convection current, namely it is the NSA.

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[17] This approximation was used independently by Liouville and Green. In quantum mechanics this approximation is known as the Wentzel–Kramers–Brillouin (WKB) approximation. However, we citing [15], "the contribution of these authors was not the construction of the approximation (which was already known), but the determination of connection formulas for linking exponential and oscillatory LG approximations across a turning point on the real axis".